4

MATHEMATICAL MODEL OF CI ENGINE

4.1 Introduction

The computational analytical approach is used for the prediction of combustion, engine performance, and emissions. The quasi-dimensional thermodynamic simulation model has been used to simulate closed power cycle of CI engine comprising, injection timing, delay period, combustion and expansion. The models developed by Whitehouse and Sareen [216] and Kumar et al. [217] are being applied to simulate the diesel engine working process and its spray mixing model. This model divides the mixture charge into burnt and unburnt zones; the burned zone corresponds to burnt fuel and unburned zone corresponds to fuel surrounding with air mixture. After injection, the ignition-delay period was calculated with respect to consuming 0.001 of the total volume of vaporized and mixed with air as spray nuclei [218] as similar to Pre-SI engine combustion. The assumed spherical spray (burning) nuclei propagation in the auto burn region inside the cylinder are simulated with respect to crank angle and corresponding heat transfer from burned and unburned [219] till the end of combustion where the volume of fresh charge V_m is just negative. Once combustion is completed, the variables are organized for a single-zone calculation. Modified empirical relations have been used to estimate burning duration as a function of equivalence ratio, speed, compression ratio, injection timing and calorific value of fuel. Heat transfer between the burned and unburned zone was neglected and the heat transfer from cylinder content to the wall has been predicted with semi-empirical correlation developed by WJD Annand [220]. The FORTRAN based

computational simulation was used to calculate with respect to crank angle of unburned and burned temperature, pressure, burned and unburned mass, volume and 12 combustion species with respect to crank angle. The variables were integrated and solved with forth order Runge-Kutta numerical method and numerical solution by Newton Raphson technique. In the numerical model following assumption and approximation were considered-

- Integrated area for the heat transfer from burned and unburned spray (burning) nuclei auto burn region inside the cylinder is assumed to govern with Wiebe function.
- During fuel injection and combustion homogeneous conditions throughout the combustion chamber, and ideal gas behavior.
- Air entrainment due to shearing action of fuel spray
- Combustion does not produce additional air entrainment.
- At any time pressure throughout the cylinder is uniform.
- The negligible volume occupied by auto burning nuclei in the reaction zone.
- Except nitrogen for species, the burned gases are at complete thermodynamic equilibrium.
- The unburned gas is frozen at its original composition.
- Both burned and unburned gases have uniform local specific heat, and changes with temperature polynomically.
- There is no heat transfer between burned and unburned zone.

The complete cycle calculation includes two main cycles

- ❖ Gas exchange cycle (includes intake and exhaust process)
- ❖ Power cycle

In this computational simulation program, the main concentration has been applied in power cycle, .i.e. processing between inlet valve close (IVC) to exhaust valve open (EVO).

4.2 Power Cycle

Power cycle occurs when inlet and exhaust valves are closed. It consists of following processes:

- ➢ Compression
- ➢ Combustion
- ➢ Expansion

4.2.1 Compression

Compression started from IVC and the trapped state includes fresh charge and residual charge of the previous cycle [221]. Computational modelling simulates 20 power cycles for the establishment of species fraction of the exhaust through Newton-Raphson method. During compression, charges and residual species are assumed in freeze condition. Pressure variation with crank angle inside the combustion chamber during compression is govern by the following equation-

$$\frac{dp}{d\theta}=\left[\frac{R}{C_v}\frac{dQ}{d\theta}-\frac{pdV}{d\theta}\left(\frac{R}{C_v}+1\right)\right]\times\frac{1}{V} \tag{4.1}$$

Where, V is the instantaneous volume $\left(\frac{\pi}{4}D^2 r\left[(1-\cos\theta)+\frac{L}{r}-\sqrt{\frac{L^2}{r^2}-\sin^2\theta}\right]\right)$ of the cylinder and $\frac{dV}{d\theta}$ is the change in instantaneous cylinder volume with respect to cranke angle, given as

$$\frac{dV}{d\theta}=\frac{\pi}{4}D^2 r\times Sin\theta\left\{1+\frac{Cos\theta}{\sqrt{\frac{L^2}{r^2}-\sin^2\theta}}\right\} \tag{4.2}$$

And at the same time change in temperature during compression is calculated by the equation

$$\frac{dT}{d\theta}=T\left(\frac{1}{V}\frac{dV}{d\theta}+\frac{1}{p}\frac{dp}{d\theta}\right) \tag{4.3}$$

Where, Q is the heat transfer from the gas to the wall is calculated by using Annand's equation [220].

$$\frac{Q}{F}=\frac{a_c K_q}{D}(R_e)^{b_c}(T_m-T_w)+c_c\left(T_m^4-T_w^4\right) \tag{4.4}$$

Where: a_c, b_c and c_c are Annand's constant values, $a_c=0.4$, $b_c=0.7$, $c_c=4.3\times10^{-9}$

F is the area of cylinder walls, D is the cylinder bore, R_e is the Reynolds number,

K_q is the thermal conductivity, $K_q=\frac{C_p\mu}{0.7}$

T_m is the temperature of unburned charge/products,

T_w is the cylinder walls temperature.

Reversible work done by reciprocating piston is

$$\frac{dW}{d\theta} = p\frac{dV}{d\theta} \tag{4.5}$$

As the compression process is continues the variables are incremented by using following equation.

$$X_{n+1} = X_n + \frac{dX}{d\theta}.\Delta\theta \tag{4.6}$$

Where, 'X' is any variable and dX is the incremented of variable X during angle step, which is calculated by the fourth order Runge-Kutta method.

4.2.2 Combustion

After injection of fuel the delay period is calculated with empirical relation used by CD Rakopoulos et al.[154]. In this stage, the state of gas inside the cylinder is calculated, applying the first law of thermodynamics for a closed system is:

$$\frac{dQ}{d\theta} = \frac{dE}{d\theta} + \frac{dW}{d\theta} \tag{4.7}$$

Where, E is total internal energy of the whole system include unburned and burned gases

$$E = m_u e_u + m_b e_b \tag{4.8}$$

And the total internal energy variation corresponding to crank angle equation-

$$\frac{dE}{d\theta} = m_u \frac{de_u}{d\theta} + e_u \frac{dm_u}{d\theta} + m_b \frac{de_b}{d\theta} + e_b \frac{dm_b}{d\theta} \tag{4.9}$$

The $dm_b/d\theta$, is burned mass fraction and, $dm_u/d\theta$ unburned mass of a total mass ($m=m_u+m_b$). The rate of burning of fuel and corresponding area of total heat transfer

$dQ/d\theta$ to cylinder wall from two zone (burned and unburned) are governed by Wiebe function.

$$\frac{dm_b}{d\theta} = m\frac{dx_b}{d\theta} \tag{4.10}$$

$$x_b = 1 - \exp\left[-a\left(\frac{\theta - \theta_s}{\theta_d}\right)^n\right] \tag{4.11}$$

$$\frac{dx_b}{d\theta} = (1 - x_b)\frac{an}{\theta_d}\left(\frac{\theta - \theta_s}{\theta_d}\right)^{n-1} \tag{4.12}$$

Where,

x_b is the mass fraction of fuel burnt at given crank angle θ,

θ_s is the start of combustion,

a is the Weibe efficiency factor (for x_{max} assumed value is 6.908),

n is the Weibe form factor (for x_{max} assumed value is 3.0)

and, θ_d is the burning duration

(a) Development of an empirical correlation for burning duration

Burning duration (θ_d), is an important measure to optimize performance and emission of an engine. It is a function of equivalence ratio (ER), compression ratio (CR), speed (N), injection timing (θ_{inj}) and calorific value of fuel. The burning duration was taken as the crank angle interval between start of burning to end of burning (last part of the charge). The following equation is the modified empirical relation and developed for CI engine. It has developed on the basis of the function of operating parameters and represented by

$f_1(CR)$, $f_2(N)$, $f_3(ER)$, $f_4(\theta_{inj})$ *and* $f_5(Blend)$. Thus the general form of burning duration can be expressed as:

$$\theta_d(CR, N, \mathrm{ER}, \theta_{inj}, Blend) = f_1(CR) \times f_2(N) \times f_3(\mathrm{ER}) \times f_4(\theta_{inj}) \times f_5(Blend) \times \theta_{d1} \tag{4.13}$$

To determine the function includes in equation 4.13, all of the operating parameters (variables) divided by their initial values such as CR_{ref}, N_{ref}, ER_{ref}, and $\theta_{inj.ref}$. The approximate functions $f_1(CR)$, $f_2(N)$, $f_3(ER)$ and $f_4(\theta_{inj})$ can be evaluated by applying a curve fitting method with the used of numerical value of burning duration (θ_d) for different values of *CR, N, ER,* θ_{inj}. The following second degree polynomial equations have been derived.

$$f_1(CR) = 3.46 - 3.42\left(\frac{CR}{CR_{ref}}\right) + 0.98\left(\frac{CR}{CR_{ref}}\right)^2 \tag{4.14}$$

$$f_2(N) = 0.76 + 0.30\left(\frac{N}{N_{ref}}\right) - 0.03\left(\frac{N}{N_{ref}}\right)^2 \tag{4.15}$$

$$f_3(\mathrm{ER}) = 4.21 - 5.65\left(\frac{\mathrm{ER}}{\mathrm{ER}_{\mathrm{ref}}}\right) + 2.40\left(\frac{\mathrm{ER}}{\mathrm{ER}_{\mathrm{ref}}}\right)^2 \tag{4.16}$$

$$f_4(\theta_{\mathrm{inj}}) = 0.64 - 0.26\left(\frac{\theta_{\mathrm{inj}}}{\theta_{\mathrm{inj.ref}}}\right) + 0.10\left(\frac{\theta_{\mathrm{inj}}}{\theta_{\mathrm{inj.ref}}}\right)^2 \tag{4.17}$$

$$f_5(Blend) = 1.07 + 0.46\left(\frac{Blend}{100}\right) - 0.52\left(\frac{Blend}{100}\right)^2 \tag{4.18}$$

And, for the known value of reference operating parameters CR_{ref}=12, N_{ref} *=1000 rpm,* ER_{ref}= 1.0, $\theta_{inj.ref}$ = −30 ^{o}CA, burning duration (θ_{d1}) is 45^{o} CA.

Figure 4.1 shows the comparison of the computed burning duration by using the empirical correlation (Equation 4.13) and experimental value given by T.A. Kumar et al. [222] with compression ratio. There is a good agreement between computed with experimental trend and value with 0.30% error. Figure 4.2 shows the variation of burning duration calculated by using the empirical correlation at different injection timing and compared with experimental results given by A.K. Agarwal et al. [223]. Figure shows the good agreement between burning duration results obtained from empirical equation and experimental value with 1.34% error. Similarly, figure 4.3 shows the comparison of the calculated burning duration with using the empirical correlation and experimental value obtained by Hosamani and Katti [224] at different biodiesel blends, and found good agreement between computed and experimental results with 1.78% error. Thus, it proves that the present computational model is capable of simulation, and further, it can be used for prediction of engine performance.

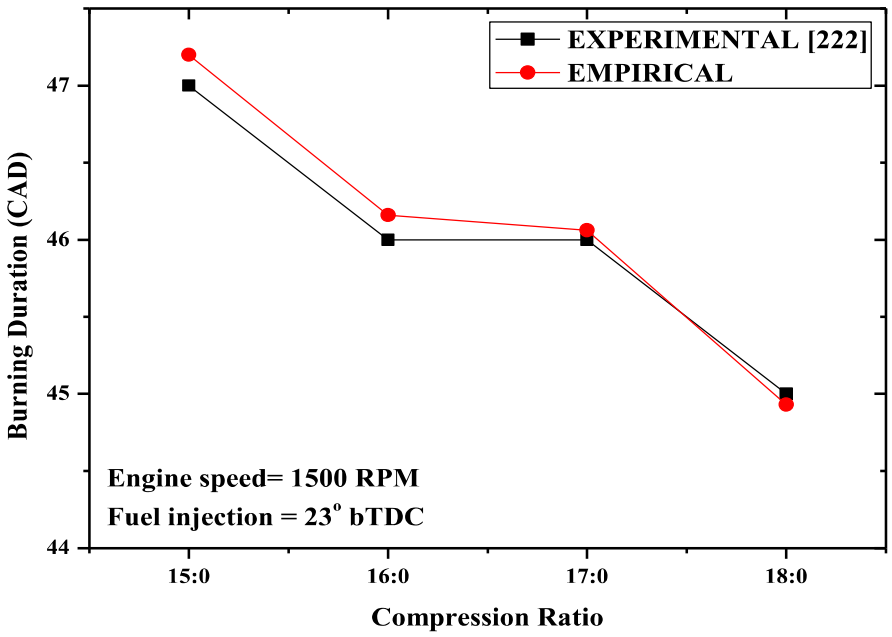

Figure 4.1: Variation of burning duration with compression ratio

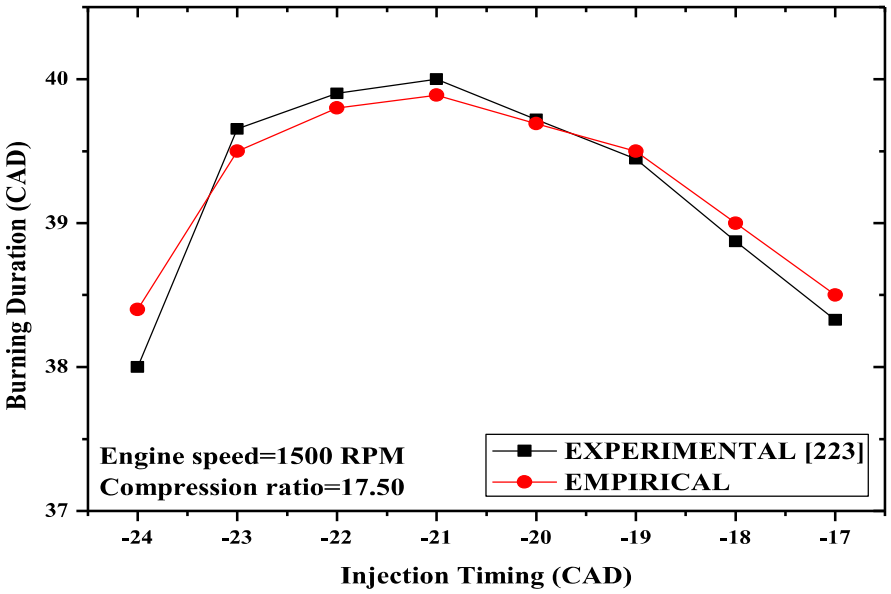

Figure 4.2: Variation of burning duration with injection timing

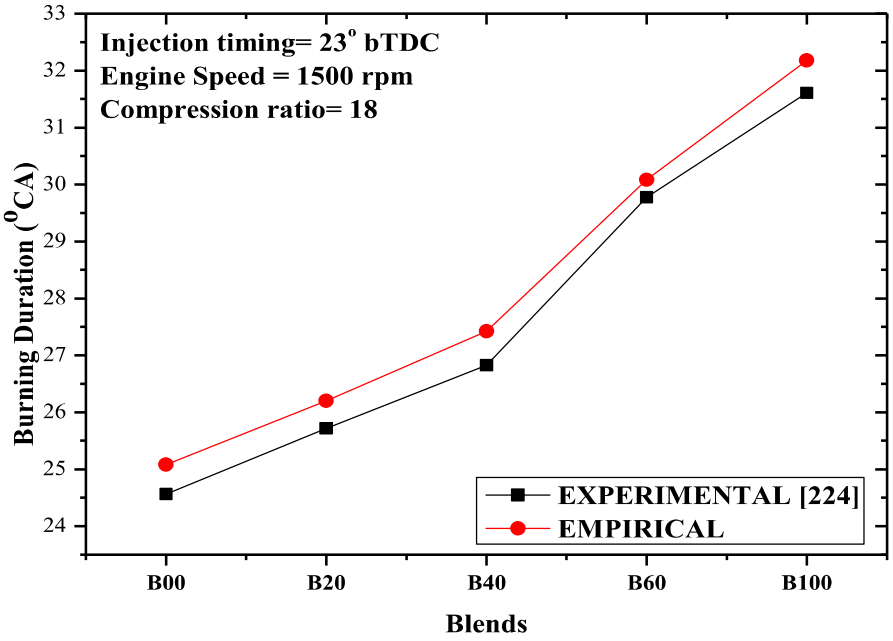

Figure 4.3: Variation of burning duration with biodiesel blends

(b) Initial combustion temperature

Initial product temperature is required to initiate the combustion process. The following expressions was given by Annand, taken from the reference [219] are being used to guess the first value of product temperature.

$$T_b = T_u + 2500 * \phi * f_i \qquad \text{for } \phi \leq 1.0 \qquad (4.19)$$

$$T_b = T_u + 2500 * \phi * f_i - 700(\phi - 1.0) f_i \qquad \text{for } \phi > 1.0 \qquad (4.20)$$

The air (unburned) temperature at the end of compression is used to calculate the first product temperature. This is done by balancing the specific internal energy of unburned mixture at guessed temperature and air at end compression with iterative technique.

Initially, a fixed product volume V_b ($=10^{-3}$ *cylinder volume) is assumed for commencement of two zone (burned and unburned) combustion. The two zone combustion is started only when the burnt volume calculated on the basis of Wiebe burning rate.

(c) Initiation of the two-zone calculation

For two zone calculation a three sequential method is adopted by steps A, B and C which is depicted in figure 4.4.

Step-A: Compression without combustion

In process 'A', it is assumed that the cylinder content ('u' unburned mixture) undergoes compression (V_1 to V_2) with heat loss dQ_u (combustion is not initiated). The condition at the end of process becomes,

$$T_u^{'} = T_{u_1}\left(\frac{V_1}{V_2}\right)^{R_u/C_{vu}} - \frac{dQ_u}{mC_{vu}} \tag{4.21}$$

$$p^{'} = \frac{p_1 V_1 T_u^{'}}{V_2 T_{u_1}} \tag{4.22}$$

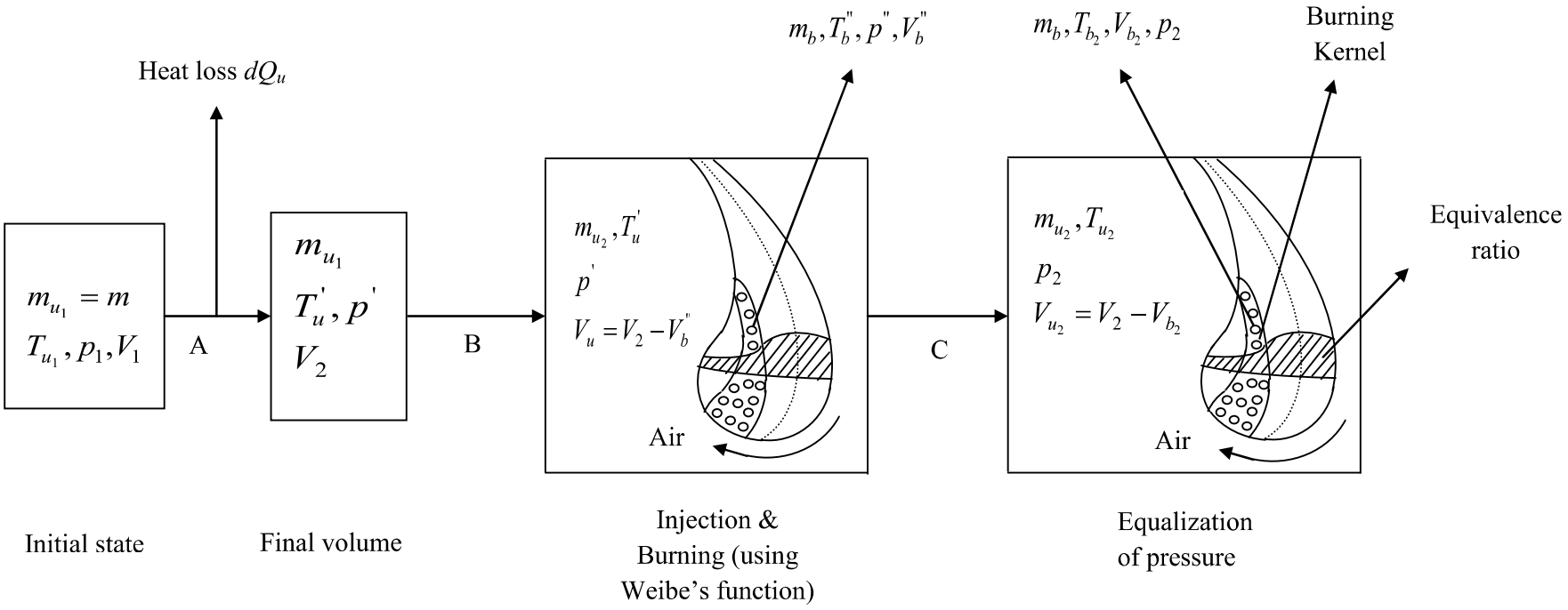

Figure 4.4: Basis of flame initiation process

Step-B: Appearance of flame nucleus

After finishing the process 'A' it is assumed that thin burning kernel spontaneously appears in the cylinder. In process 'B' the assumption is that the flame nucleus is formed by constant specific volume combustion, which results in a high pressure and temperature in the product region. Since the combustion is at constant volume the unburned mixture zone is maintained at constant temperature and pressure T'_u and p' respectively.

The temperature of product in the flame nucleus (T_b'') is calculated by Annand expression, and the pressure in the burnt kernel can be calculated as follows,

$$p'' = \frac{R_b T_b''}{R_u T_u'} p' \tag{4.23}$$

And, the mass of product is, $$m_b = \frac{2\pi r^3}{3V_2} m \tag{4.24}$$

Where m is the total mass trapped in the cylinder. Mass of the mixture remaining after process 'B' is

$$m_{u_2} = m - m_b \tag{4.25}$$

Total internal energy $$E = m_{u_2} e_u' + m_b e_b'' \tag{4.26}$$

Step-C: Pressure equalization

The assumption of constant specific volume combustion in process B produces a pressure differences between burned and unburned area. This is physically impossible so a further process is required to equalize the pressure throughout the cylinder. In process 'C' it is assumed that pressure equalization occurs adiabatically at constant cylinder volume, thus

the process is one of the constant internal energy, E, because although the products and mixture zones do work on each other, there is no net work done by the whole system.

Equating the total internal energy before and after process 'C'

$$m_{u_2} e_u^{'} + m_b e_b^{"} = m_{u_2} e_{u_2} + m_b e_{b_2} \tag{4.27}$$

$$m_{u_2} C_{vu} T_u^{'} \left[\frac{T_{u_2}}{T_u^{'}} - 1 \right] = m_b^{"} C_{vb} T_b^{"} \left[1 - \frac{T_{p_2}}{T_b^{"}} \right] \tag{4.28}$$

For the reversible adiabatic process

$$\frac{T_{u_2}}{T_u^{'}} = \left(\frac{p_2}{p^{'}} \right)^{\frac{k_u - 1}{k_u}} \tag{4.29}$$

and,

$$\frac{T_{b_2}}{T_b^{"}} = \left(\frac{p_2}{p^{"}} \right)^{\frac{k_b - 1}{k_b}} \tag{4.30}$$

and, also

$$\frac{p_2}{p^{"}} = \frac{p_2}{p^{'}} \times \frac{p^{'}}{p^{"}} = \frac{p_2}{p^{'}} \times \frac{R_u T_u^{'}}{R_b T_b^{"}} \tag{4.31}$$

Using the equation (b), (d) and (e) following relation is obtained

$$\psi - 1 = A(1 - B\psi^{\alpha}) \tag{4.32}$$

Where, $\psi = \frac{T_{u_2}}{T_u^{'}}, \alpha = \frac{k_u}{k_u - 1} \times \frac{k_b - 1}{k_b}$

$$A = \frac{m_b C_{vb} T_b^{"}}{m_{u_2} C_{vu} T_m^{'}}, \; B = \left(\frac{R_u T_u^{'}}{R_b T_b^{"}} \right)^{\frac{k_b - 1}{k_b}}$$

The equation (4.32) solve for ψ with an iterative technique.

4.2.3 Expansion (two-zone expansion)

The temperature and pressure of burned and unburned mixture can be obtained by applying the first law of thermodynamics, energy equation, flame speed and the geometry of burned zone in relation to the combustion chamber.

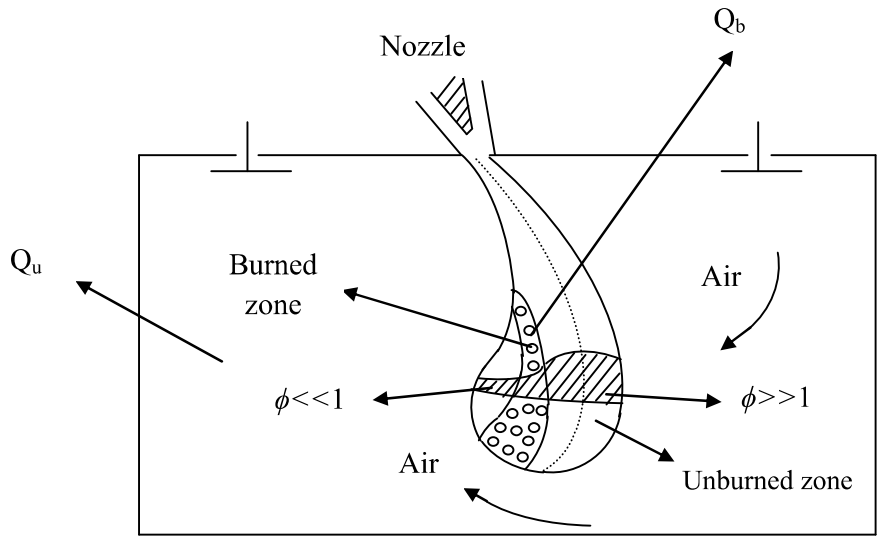

Figure 4.5: System with two zones

Apply the first law of thermodynamic for whole closed system (unburned and burned zone)

$$\frac{dQ}{d\theta} = \frac{dE}{d\theta} + \frac{dW}{d\theta} \tag{4.33}$$

Where, Q is heat transfer from burned and unburned region (Q_u and Q_b) to the cylinder wall, W is work transfer through piston displacement (pdV) by burned and unburned volume and E, total internal energy of the whole system (unburned and burned zone).

$$E = m_u e_u + m_b e_b \tag{4.34}$$

Differentiate the equation (4.34) with respect to crank angle, yield

$$\frac{dE}{d\theta} = m_u \frac{de_u}{d\theta} + e_u \frac{dm_u}{d\theta} + m_b \frac{de_b}{d\theta} + e_b \frac{dm_b}{d\theta} \tag{4.35}$$

If $\frac{dm_u}{d\theta} = -\frac{dm_b}{d\theta}$, i.e., rate of combustion of unburned mass is equal to rate of decreasing the product mass (dm_b).

Put the $\frac{dm_u}{d\theta} = -\frac{dm_b}{d\theta}$ in equation (4.35), then

$$\frac{dE}{d\theta} = m_u \frac{de_u}{d\theta} + e_u \frac{dm_u}{d\theta} - m_b \frac{de_b}{d\theta} + e_b \frac{dm_b}{d\theta}$$

$$\frac{dE}{d\theta} = m_u \frac{de_u}{d\theta} + e_u \left(-\frac{dm_b}{d\theta} \right) - m_b \frac{de_b}{d\theta} + e_b \frac{dm_b}{d\theta}$$

$$\frac{dE}{d\theta} = \left(e_b - e_u\right)\frac{dm_b}{d\theta} + m_u \frac{de_u}{d\theta} - m_b \frac{de_b}{d\theta} \tag{4.36}$$

From equation (4.33)

$$\frac{dQ}{d\theta} = \frac{dE}{d\theta} + \frac{pdV}{d\theta} \Rightarrow \frac{dE}{d\theta} + \frac{pdV}{d\theta} - \frac{dQ}{d\theta} = 0 \tag{4.37}$$

Where, $$\frac{dV}{d\theta} = \frac{dV_u}{d\theta} + \frac{dV_b}{d\theta} \tag{4.38}$$

Equation of state, $$pV = mRT \tag{4.39}$$

Therefore, $$V_u = \frac{m_u R_u T_u}{p}, V_b = \frac{m_b R_b T_b}{p} \tag{4.40}$$

Then, differentiating the equation (4.40) with respect to crank angle, yield

$$\frac{dV_u}{d\theta} = \frac{m_u R_u}{p}\frac{dT_u}{d\theta} + \frac{m_u R_u}{p}\frac{dm_u}{d\theta} - \frac{m_u R_u T_u}{p^2}\frac{dp}{d\theta} \tag{4.41}$$

$$\frac{dV_b}{d\theta} = \frac{m_b R_b}{p}\frac{dT_b}{d\theta} + \frac{m_b R_b}{p}\frac{dm_b}{d\theta} - \frac{m_b R_b T_b}{p^2}\frac{dp}{d\theta} \tag{4.42}$$

Combined the equation put the value $\frac{dV_u}{d\theta} and \frac{dV_b}{d\theta}$ in equation (4.38), yield

$$\frac{dV}{d\theta} = \left[\frac{m_u R_u}{p}\frac{dT_u}{d\theta} + \frac{m_u R_u}{p}\frac{dm_u}{d\theta} - \frac{m_u R_u T_u}{p^2}\frac{dp}{d\theta}\right] + \left[\frac{m_b R_b}{p}\frac{dT_b}{d\theta} + \frac{m_b R_b}{p}\frac{dm_b}{d\theta} - \frac{m_b R_b T_b}{p^2}\frac{dp}{d\theta}\right]$$

$$\frac{dV}{d\theta} = \left[\frac{m_u R_u}{p}\frac{dT_u}{d\theta} + \frac{m_u R_u}{p}\left(-\frac{dm_b}{d\theta}\right) - \frac{m_u R_u T_u}{p^2}\frac{dp}{d\theta}\right] + \left[\frac{m_b R_b}{p}\frac{dT_b}{d\theta} + \frac{m_b R_b}{p}\frac{dm_b}{d\theta} - \frac{m_b R_b T_b}{p^2}\frac{dp}{d\theta}\right]$$

$$\frac{dV}{d\theta} = \left(\frac{V_b}{m_b} - \frac{V_u}{m_u}\right)\frac{dm_u}{d\theta} + \frac{m_u R_u}{p}\frac{dT_u}{d\theta} + \frac{m_b R_b}{p}\frac{dT_b}{d\theta} - \frac{(V_u + V_b)}{p}\frac{dp}{d\theta}$$

$$\frac{dV}{d\theta} = \left(\frac{V_b}{m_b} - \frac{V_u}{m_u}\right)\frac{dm_u}{d\theta} + \frac{m_u R_u}{p}\frac{dT_u}{d\theta} + \frac{m_b R_b}{p}\frac{dT_b}{d\theta} - \frac{V}{p}\frac{dp}{d\theta} \tag{4.43}$$

From equation (4.33), First law of thermodynamic for whole system:-

$$\frac{dQ}{d\theta} = \frac{dE}{d\theta} + \frac{dW}{d\theta} \Rightarrow \frac{dE}{d\theta} = \frac{dQ}{d\theta} - \frac{pdV}{d\theta} \tag{4.44}$$

Equation (4.44) used for unburned mixture specific internal energy

$$\frac{de_u}{d\theta} = \frac{1}{m_u}\frac{dQ_u}{d\theta} - \frac{p}{m_u}\frac{dV_u}{d\theta} \tag{4.45}$$

or, $$C_{vu}\frac{dT}{d\theta} = \frac{1}{m_u}\frac{dQ_u}{d\theta} - \frac{p}{m_u}\frac{dV_u}{d\theta} \qquad (\text{as, } e = C_v T)$$

From the equation of state

$$pV = RT \Rightarrow V = \frac{RT}{P} \tag{4.46}$$

Differentiating the equation (4.46) with respect to crank angle, yield

$$\frac{dV}{d\theta}=\frac{R}{P}\frac{dT}{d\theta}-\frac{RT}{P^2}\frac{dp}{d\theta}=\frac{V}{T}\frac{dT}{d\theta}-\frac{V}{P}\frac{dp}{d\theta}=V\left(\frac{1}{T}\frac{dT}{d\theta}-\frac{1}{P}\frac{dp}{d\theta}\right) \tag{4.47}$$

(a) Unburned mixture temperature

We know that the specific internal energy $(e=C_vT)$, and then from (4.45) and (4.47)

$$C_{vu}\frac{dT_u}{d\theta}=\frac{1}{m_u}\frac{dQ_u}{d\theta}-\frac{pV_u}{m_u}\left(\frac{1}{T}\frac{dT_u}{d\theta}-\frac{1}{p}\frac{dp}{d\theta}\right)\Rightarrow\frac{dT_u}{d\theta}\left(C_{vu}+\frac{pV_u}{T}\right)=\frac{1}{m_u}\frac{dQ_u}{d\theta}+\frac{V_u}{m_u}\frac{dp}{d\theta}\Rightarrow$$

$$\frac{dT_u}{d\theta}\left(C_{vu}+R_u\right)=\frac{1}{m_u}\frac{dQ_u}{d\theta}+\frac{V_u}{m_u}\frac{dp}{d\theta}\Rightarrow C_{pu}\frac{dT_u}{d\theta}=\frac{1}{m_u}\frac{dQ_u}{d\theta}+\frac{V_u}{m_u}\frac{dp}{d\theta}\Rightarrow$$

$$\frac{dT_u}{d\theta}=\frac{1}{m_uC_{pu}}\left(V_u\frac{dp}{d\theta}+\frac{dQ_u}{d\theta}\right) \tag{4.48}$$

Where, Q_u is the heat transfer from the unburned mixture, and assumed that it is uniformly distributed throughout the unburned mixture and V_u is the volume of the unburned mixture.

(b) Product (burned) temperature

To find the product temperature; put the value $\frac{dT_u}{d\theta}$ from equation (4.48) in equation (4.43)

$$\frac{dT_b}{d\theta}=\frac{p}{m_bR_b}\left[\frac{dV}{d\theta}-\left(\frac{V_b}{m_b}-\frac{V_u}{m_u}\right)\frac{dm_b}{d\theta}-\frac{m_uR_u}{p}\frac{dT_u}{d\theta}+\frac{m_bR_b}{p}\frac{dT_b}{d\theta}+\frac{V}{p}\frac{dp}{d\theta}\right]\Rightarrow$$

$$\frac{dT_b}{d\theta}=\frac{p}{m_bR_b}\left[\frac{dV}{d\theta}-\left(\frac{R_bT_b}{p}-\frac{R_uT_u}{p}\right)\frac{dm_b}{d\theta}-\frac{m_uR_u}{p}\left(\frac{1}{m_uC_{pu}}\frac{dQ_u}{d\theta}+\frac{v_u}{m_uC_{pu}}\frac{dp}{d\theta}\right)+\frac{V}{P}\frac{dp}{d\theta}\right]\Rightarrow$$

$$\frac{dT_b}{d\theta}=\frac{p}{m_bR_b}\left[\frac{dV}{d\theta}-\left(\frac{R_bT_b}{p}-\frac{R_uT_u}{p}\right)\frac{dm_b}{d\theta}-\frac{m_uR_u}{p}\frac{1}{m_uC_{pu}}\frac{dQ_u}{d\theta}-\frac{m_uR_u}{p}\frac{v_u}{m_uC_{pu}}\frac{dp}{d\theta}+\frac{V}{P}\frac{dp}{d\theta}\right]\Rightarrow$$

$$\frac{dT_b}{d\theta}=\frac{p}{m_bR_b}\left[\frac{dV}{d\theta}-\left(\frac{R_bT_b}{p}-\frac{R_uT_u}{p}\right)\frac{dm_b}{d\theta}-\frac{R_u}{pC_{pu}}\frac{dQ_u}{d\theta}-\frac{R_uV_u}{pC_{pu}}\frac{dp}{d\theta}+\frac{V}{p}\frac{dp}{d\theta}\right] \tag{4.49}$$

(c) Cylinder pressure

Putting the value of $dE/d\theta$ from equation (4.36) in equation (4.37), yield

$$(e_b-e_u)\frac{dm_b}{d\theta}+m_u\frac{de_u}{d\theta}-m_b\frac{de_b}{d\theta}+\frac{pdV}{d\theta}-\frac{dQ}{d\theta}=0 \tag{4.50}$$

As we know that the specific internal energy $(e)=C_vT$, then equation (4.50) becomes:-

$$(e_b-e_u)\frac{dm_b}{d\theta}+m_uC_{vu}\frac{dT_u}{d\theta}-m_bC_{vb}\frac{dT_b}{d\theta}+\frac{pdV}{d\theta}-\frac{dQ}{d\theta}=0 \tag{4.51}$$

Put the value of $\frac{dT_u}{d\theta}and\frac{dT_b}{d\theta}$ from equation (4.48) and (4.49) in equation (4.51)

$$(e_b-e_u)\frac{dm_b}{d\theta}+m_uC_{vu}\left(\frac{1}{C_{pu}m_u}\frac{dQ_u}{d\theta}+\frac{V_u}{m_uC_{pu}}\frac{dp}{d\theta}\right)-m_bC_{vb}\left\{\frac{p}{m_bR_b}\left[\begin{array}{l}\frac{dV}{d\theta}-\left(\frac{R_bT_b}{p}-\frac{R_uT_u}{p}\right)\frac{dm_b}{d\theta}\\-\frac{R_u}{pC_{pu}}\frac{dQ_u}{d\theta}-\frac{R_uV_u}{pC_{pu}}\frac{dp}{d\theta}\\+\frac{V}{p}\frac{dp}{d\theta}\end{array}\right]\right\}$$

$$+\frac{pdV}{d\theta}-\frac{dQ}{d\theta}=0\Rightarrow$$

$$(e_b-e_u)\frac{dm_b}{d\theta}+\frac{m_uC_{vu}}{C_{pu}m_u}\frac{dQ_u}{d\theta}+\frac{m_uC_{vu}V_u}{m_uC_{pu}}\frac{dp}{d\theta}-m_bC_{vb}\left\{\frac{p}{m_bR_b}\left[\begin{array}{l}\frac{dV}{d\theta}-\left(\frac{R_bT_b}{p}-\frac{R_uT_u}{p}\right)\frac{dm_b}{d\theta}-\\\frac{R_u}{pC_{pu}}\frac{dQ_u}{d\theta}-\frac{R_uV_u}{pC_{pu}}\frac{dp}{d\theta}+\\\frac{V}{p}\frac{dp}{d\theta}\end{array}\right]\right\}+$$

$$\frac{pdV}{d\theta}-\frac{dQ}{d\theta}=0\Rightarrow$$

$$(e_b - e_u)\frac{dm_b}{d\theta} + \frac{C_{vu}}{C_{pu}}\frac{dQ_u}{d\theta} + \frac{C_{vu}V_u}{C_{pu}}\frac{dp}{d\theta} - \frac{C_{vb}p}{R_b}\frac{dV}{d\theta} - \left(\frac{R_bT_b}{p} - \frac{R_uT_u}{p}\right)\frac{C_{vb}p}{R_b}\frac{dm_b}{d\theta} - \frac{C_{vb}p}{R_b}\frac{R_u}{pC_{pu}}\frac{dQ_u}{d\theta} -$$
$$\frac{C_{vb}p}{R_b}\frac{R_uV_u}{pC_{pu}}\frac{dp}{d\theta} + \frac{C_{vb}p}{R_b}\frac{V}{p}\frac{dp}{d\theta} + \frac{pdV}{d\theta} - \frac{dQ}{d\theta} = 0 \Rightarrow$$

$$(e_b - e_u)\frac{dm_b}{d\theta} - (R_bT_b - R_uT_u)\frac{C_{vb}}{R_b}\frac{dm_b}{d\theta} + \frac{dp}{d\theta}\left(\frac{C_{vu}V_u}{C_{pu}} - \frac{C_{vb}}{R_b}\frac{R_uV_u}{C_{pu}} + \frac{C_{vb}p}{R_b}V\right) + \frac{dQ_u}{d\theta}\left(\frac{C_{vu}}{C_{pu}} - \frac{C_{vb}}{R_b}\frac{R_u}{C_{pu}}\right)$$
$$+ \frac{pdV}{d\theta}\left(\frac{C_{vb}}{R_b} + 1\right) - \frac{dQ}{d\theta} = 0 \Rightarrow$$

$$\frac{dm_b}{d\theta}\left[(e_b - e_u) - \left(T_b - \frac{R_u}{R_b}T_u\right)\right] + \frac{dp}{d\theta}\left(\frac{C_{vu}V_u}{C_{pu}} - \frac{C_{vb}}{R_b}\frac{R_uV_u}{C_{pu}} + \frac{C_{vb}p}{R_b}V\right) + \frac{dQ_u}{d\theta}\left(\frac{C_{vu}}{C_{pu}} - \frac{C_{vb}}{R_b}\frac{R_u}{C_{pu}}\right) +$$
$$\frac{pdV}{d\theta}\left(\frac{C_{vb}}{R_b} + 1\right) - \frac{dQ}{d\theta} = 0 \Rightarrow$$

$$\frac{dm_b}{d\theta}\left[(e_b - e_u) - \left(T_b - \frac{R_u}{R_b}T_u\right)\right] + \frac{dp}{d\theta}\left(\frac{C_{vu}V_u}{C_{pu}} - \frac{C_{vb}}{R_b}\frac{R_uV_u}{C_{pu}} + \frac{C_{vb}p}{R_b}V\right) + \frac{dQ_u}{d\theta}\left(\frac{C_{vu}}{C_{pu}} - \frac{C_{vb}}{R_b}\frac{R_u}{C_{pu}}\right)$$
$$+ \frac{pdV}{d\theta}\left(\frac{C_{vb}}{R_b} + 1\right) - \frac{dQ}{d\theta} = 0 \Rightarrow$$

$$\frac{dp}{d\theta} = \frac{\left\{\frac{pdV}{d\theta}\left(\frac{C_{vb}}{R_b} + 1\right) + \frac{dm_b}{d\theta}\left[(e_b - e_u) - \left(T_b - \frac{R_uT_u}{R_b}\right)\right] + \frac{dQ_u}{d\theta}\left(\frac{C_{vu}}{C_{pu}} - \frac{C_{vb}}{R_b}\frac{R_u}{C_{pu}}\right) - \frac{dQ}{d\theta}\right\}}{\left(\frac{C_{vu}V_u}{C_{pu}} - \frac{C_{vb}}{R_b}\frac{R_uV_u}{C_{pu}} + \frac{C_{vb}p}{R_b}V\right)} \tag{4.52}$$

Where subscript u is unburned and b shows burnt zone. dQ/dθ Heat transfer from the gas to cylinder coolant wall, which is estimated by Aannad's equation [5] Runge-Kutta fourth order numerical procedure, was adopted to solve the differential equation, and the variables are incremented in order of any X variable.

$$X_{n+1} = X_n + \frac{dX}{d\theta}.\Delta\theta \tag{4.53}$$

Once combustion is completed, the variables are organized to calculate for single-zone only where only burnt and unburnt is considered. Thus, following equations have been obtained from 4.54 and 4.55 for single zone expansion (only product), to governs the pressure and temperature in the combustion chamber till the exhaust valve open.

$$\frac{dp}{d\theta} = \frac{1}{V}\left[\left(1+\frac{R_b}{C_{vb}}\right)p\frac{dV}{d\theta} - \frac{R_b}{C_{vb}}\frac{dQ}{d\theta}\right] \tag{4.54}$$

$$\frac{dT_b}{d\theta} = T_b\left(\frac{1}{V_b}\frac{dV}{d\theta} + \frac{1}{p}\frac{dp}{d\theta} - \frac{1}{m_b}\frac{dm_b}{d\theta}\right) \tag{4.55}$$

4.3 Species formation

The following H_2O, H_2, OH, H, N_2, NO, N, CO_2, CO, O_2, O and Ar twelve species are considered to be form in the combustion chamber (product) and in the exhaust gases. The polynomial coefficients of internal energy of these twelve species are used to calculate the properties of mixture at every time step. These species could reach equilibrium condition if sufficient time is allowed for the reactions to take place under a certain state [219, 225]. To determine the 12 species concentration and relative equilibrium constants following 7 chemical equilibrium equations were used.

(i) $\frac{1}{2}H_2 \Leftrightarrow H$, $K_{p_1} = \frac{x_4}{\sqrt{x_2}}p^{1/2}$ (4.56)

(ii) $\frac{1}{2}O_2 \Leftrightarrow O$ $K_{p_2} = \frac{x_{11}}{\sqrt{x_{10}}}p^{1/2}$ (4.57)

(iii) $\frac{1}{2}N_2 \Leftrightarrow N$ $K_{p_3} = \frac{x_7}{\sqrt{x_5}}p^{1/2}$ (4.58)

(iv) $2H_2O \Leftrightarrow 2H_2 + O_2$ $\qquad K_{p_4} = \dfrac{x_{10}}{\left(x_1 / x_2\right)^2} p$ (4.59)

(v) $H_2O \Leftrightarrow OH + \dfrac{1}{2}H_2$ $\qquad K_{p_5} = \dfrac{x_3}{\left(x_1 / \sqrt{x_2}\right)} p^{1/2}$ (4.60)

(vi) $CO_2 + H_2 \Leftrightarrow H_2O + CO$ $\qquad K_{p_6} = \dfrac{x_1}{x_2} \times \dfrac{x_9}{x_8}$ (4.61)

(vii) $H_2O + \dfrac{1}{2}N_2 \Leftrightarrow H_2 + NO$ $\qquad K_{p_7} = \dfrac{x_2}{x_1} \times \dfrac{x_6}{\sqrt{x_5}} p^{1/2}$ (4.62)

Criterion for chemical equilibrium can be expressed by Gibbs function as:

$$(dG)_{T,p} = 0 \tag{4.63}$$

Where specific Gibbs function is expressed as;

$$\frac{g(T)}{\bar{R}T} = a_g(1 - \ln T) - b_g T - \frac{C_g}{2}T^2 - \frac{d_g}{3}T^3 - \frac{e_g}{4}T^4 - k_g \tag{4.64}$$

Where a_g, b_g c_g, d_g, e_g and k_g are constants. Considering the seven equilibrium equation of reaction used by [225] and the value of equilibrium constant K_p was obtained by universal equation:

$$\upsilon_a A + \upsilon_a B \Leftrightarrow \upsilon_c C + \upsilon_d D \tag{4.65}$$

$$K_p = \frac{X_c^{\upsilon_c} X_d^{\upsilon_d}}{X_a^{\upsilon_a} X_b^{\upsilon_b}} \times P^{\upsilon_c + \upsilon_d - \upsilon_a - \upsilon_b} \tag{4.66}$$

$$\ln K_p = \left[\sum \left\{ \frac{\upsilon . g(T)}{\bar{R}T} \right\}_{\text{Reactant}} - \sum \left\{ \frac{\upsilon . g(T)}{\bar{R}T} \right\}_{\text{Product}} \right] - \frac{\Delta H_o}{\bar{R}T} \tag{4.67}$$

'υ' is stoichiometric coefficient, 'X', is molar fraction and 'P' is total pressure.

The calculation starts from the reaction of a hydrocarbon fuel and air, which is presented by:-

$$a(C_nH_mO_r)+\frac{a}{\phi}\left(n+\frac{m}{4}-\frac{r}{2}\right)\left[O_2+\frac{78}{21}+\frac{1}{21}A_r\right]\rightarrow X_{H_2O}H_2O+X_{H_2}H_2+X_{OH}OH+ \\ X_HH+X_{N_2}N_2+X_{NO}NO+X_NN+X_{CO_2}CO_2+X_{CO}CO+X_{O_2}O_2+X_OO+X_{A_r}A_r \quad (4.68)$$

There are 13 unknown in this equation; 12 species fraction (x_i) and number of moles of fuel (a) to produce one mole of products. Seven equations are already formulated as describe above. The five equations are obtained from fuel-air reaction equation (eq^n 4.68) by atom balance of Ar, C, H, O and N.

Argon $$x_{12}=av \quad (4.69)$$

Carbon $$x_8+x_9=aw \quad (4.70)$$

Hydrogen $$2x_1+2x_2+x_3+x_4=ax \quad (4.71)$$

Oxygen $$x_1+x_3+x_6+2x_8+x_9+2x_{10}+x_{11}=ay \quad (4.72)$$

Nitrigen $$2x_5+x_6+x_7=az \quad (4.73)$$

Where, *v, w, x, y* and *z* are denoting the number of Ar, C, H, O and N atom corresponding to one mole of fuel, and its values known from fuel-air reaction equation (eq^n 4.68). The last equation is obtained by summation of mole fraction of the component (*i*) in the product.

$$\sum_{i=1}^{q}X_i=1 \quad (4.74)$$

Where, *q* is the total number of components (twelve species in product in the cylinder and in the exhaust gases i.e. *q* = 12).

The method of solution is based on the method used by Vickland et al. modified by Annand taken from the reference [219].

4.3.1 Rate Kinetics of NO formation

The formation of Nitric Oxide and Carbon monoxide during combustion in the cylinder is non-equilibrium process. Present work comprises the rate kinetics of NO. Lavoie GA (1970) et al.[226] were developed rate of a kinematic model for NO formation. These are the seven governing equations for NO formation:

(i) $N + NO \Leftrightarrow N_2 + O \qquad K_{1f} = 3.1\times10^{10} \times e^{(-160/T)}$ (4.75)

(ii) $N + O_2 \Leftrightarrow NO + O \qquad K_{2f} = 6.4\times10^{6} \times T \times e^{(-3125/T)}$ (4.76)

(iii) $N + OH \Leftrightarrow NO + H \qquad K_{3f} = 4.2\times10^{10}$ (4.77)

(iv) $H + N_2O \Leftrightarrow N_2 + OH \qquad K_{4f} = 3.0\times10^{10} \times e^{(-5350/T)}$ (4.78)

(v) $O + N_2O \Leftrightarrow N_2 + O_2 \qquad K_{5f} = 3.2\times10^{12} \times T \times e^{(-18900/T)}$ (4.79)

(vi) $O + N_2O \Leftrightarrow NO + NO \qquad K_{6f} = K_{5f}$ (4.80)

(vii) $N_2O + M \Leftrightarrow N_2 + O + M \qquad K_{7f} = 10^{12} \times e^{(-30500/T)}$ (4.81)

Where,

M is the third body which may be any of the other species in the mixture and remains chemically unchanged during the reaction.

The rate of formation of nitric oxide is derived as follows:-

$$K_{1f}[N]_e[NO]_e = K_{1b}[N_2]_e[O]_e = R_1 \tag{4.82}$$

$$K_{2f}[N]_e[O_2]_e = K_{2b}[NO]_e[O]_e = R_2 \tag{4.83}$$

$$K_{3f}[N]_e[OH]_e = K_{3b}[NO]_e[H]_e = R_3 \tag{4.84}$$

$$K_{4f}[H]_e[N_2O]_e = K_{4b}[N_2]_e[OH]_e = R_4 \tag{4.85}$$

$$K_{5f}[O]_e[N_2O]_e = K_{5b}[N_2]_e[O_2]_e = R_5 \tag{4.86}$$

$$K_{6f}[O]_e[N_2O]_e = K_{6b}[NO]_e[NO]_e = R_6 \tag{4.87}$$

$$K_{7f}[N_2O]_e[M]_e = K_{7b}[N_2]_e[O]_e[M]_e = R_7 \tag{4.88}$$

Where,

K_{if} is the forward reaction rate of constant, and K_{ib} is the backward reaction rate of constant.

The calculation method and details are given in [218]. The total rate equation for NO is:-

$$\frac{1}{V}\frac{d}{dt}\left[[NO]V\right] = 2(1-\alpha_e^2)\left[\frac{R_1}{1+\alpha_e\dfrac{R_1}{R_2+R_3}} + \frac{R_6}{1+\dfrac{R_6}{R_4+R_5+R_7}}\right] \tag{4.89}$$

Where,

$$\alpha_e = \frac{[NO]}{[NO]_e}$$

and ‘e ‘represents the equilibrium condition.

4.3.2 CO formation

The formation of CO (carbon monoxide) is mainly due to incomplete combustion, and it forms during the intermediate stage of combustion of fuel. At the end of the expansion stroke, the formation of CO is greater than the value determines by using the equilibrium condition. The various researchers had worked on formation and decomposition of CO by rate kinetics [226].

To determine the accurate value at the exhaust introduced a multiplication factor called 'COFAC'. For the computation work using the following relations:

$$XCO = XCO_{eq} + COFAC\ (XCO_{max} - X\ CO_{eq}) \tag{4.90}$$

Where,

XCO= Concentration of corrected CO,

XCO_{eq} = Concentration of CO at equilibrium,

XCO_{max} =Maximum value of CO concentration at equilibrium condition.

And, COFAC = It is the scale factor (its value lies between 0 and 1).

The value '0' and '1' shows the instantaneous equilibrium state and frozen at the peak value of CO.

4.4 Validation of mathematical modelling

Figure 4.6 shows the validation of P-θ for experimental and computational results when engine fuelled with pure diesel at compression ratio 16. The experimental works have been conducted on VCR engine run with diesel. The engine details are given in table 3.3. The different results of P-θ obtained with the experiment work, among these P_{avg} at 215

CAD (35^{o} aBDC) considered as trap pressure (P_{trap}). The natures of P-θ for computational results are following nearly same trends as experimental with 5.67% error.

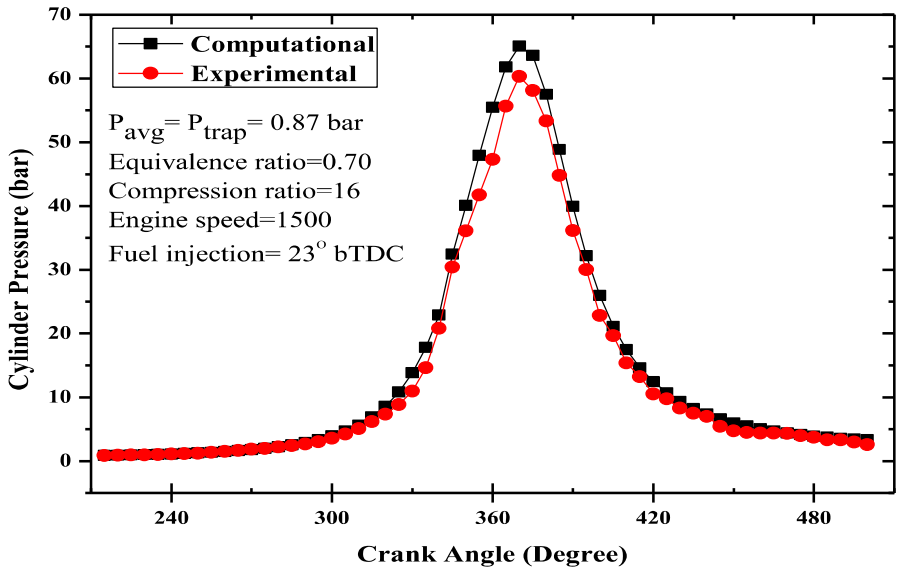

Figure 4.6: Validation of cylinder pressure and crank angle

Burning duration is an important phenomenon to achieve optimum performance in term of brake mean efective pressure (BMEP), and brake power (BP). The empirical relation for burning duration is developed in this chaper, equation 4.13. Figure 4.7 and 4.8 shows comparison of computed results (BMEP and Brake Power) with experimental value obtained by Atul Dhar et al. [227] and E. Rajasekar et al. [228] for burning duration, and shows good agreement between computed with experimental trend and value with 0.43% and 1.81 % error. There are slight variation in results due to the taking some assumption during mathematical formulation for computational program. On the basis of validation, following results (BP, IP, BSFC, ISFC, BMEP, IMEP, Pmax and NO emission) have been obtained using the computational program, in chapter 6.

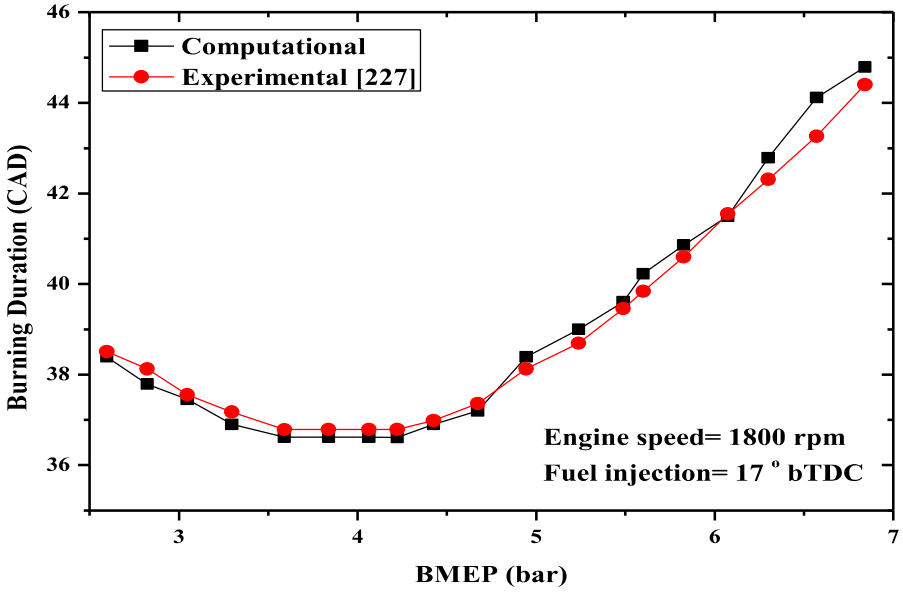

Figure 4.7: Burning duration vs BMEP

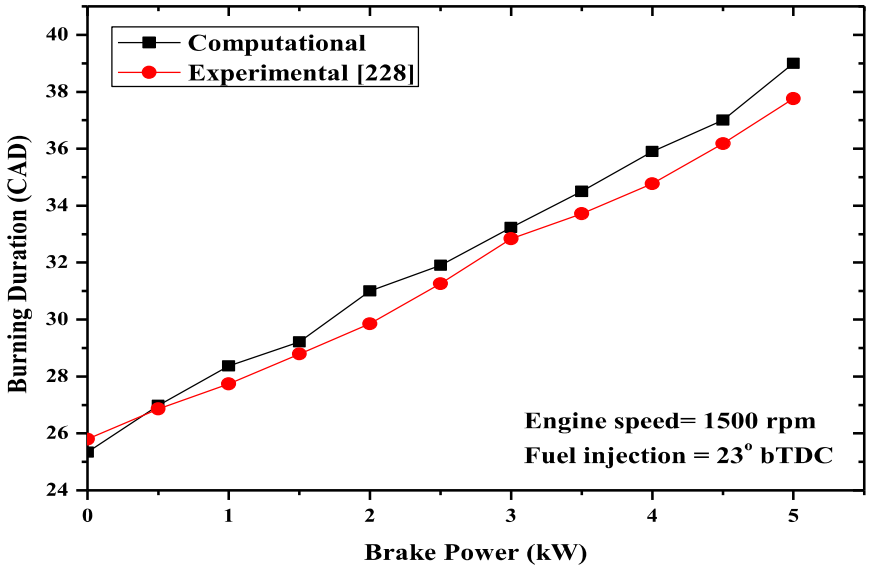

Figure 4.8: Burning duration vs Brake Power

4.5 Main programme

In the present work, computational simulation model (FORTRAN code) has been used to simulate a four stroke power cycle of CI engine fuelled with diesel and biodiesel. The present model is based on quasi-dimentional (burned and unburned region) to simulate compression, combustion and expansion processes of CI engine power cycles. The brief of simulation programming is shown in figure 4.9 and, the details of main programming and subroutines are given in the appendices [B and C].

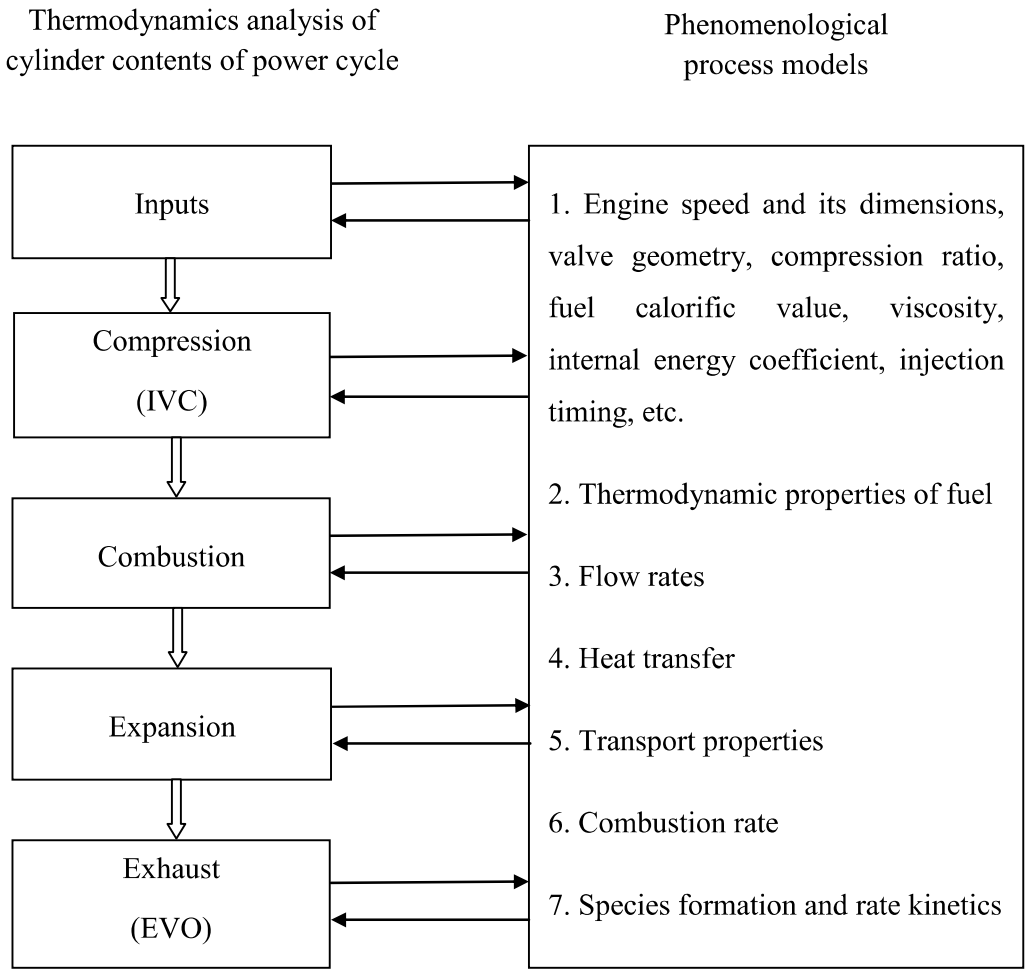

Figure 4.9: Flow diagram of quasi-dimensional thermodynamic-based simulation of CI engine operating cycle